

Disorder and Interactions on a 1D Chain

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1. Introduction

It is well established that in the presence of disorder electron wavefunctions can become localized. Considerable numerical work has been carried out for non-interacting systems with results reaching a reasonable consensus: theory and experiment are in general qualitative agreement. However, in 3D the determined value of the universal critical exponent is markedly larger than the empirically measured value.¹⁾ This seems to suggest that an essential factor is missing from calculations: the obvious candidate is the electron-electron interaction. Furthermore, some have claimed to observe a Metal-Insulator transition in 2D contrary to the widely accepted scaling theory of Anderson localization.²⁾ This is often accredited to the effect of interactions. Hence during the last 10 years attention has been switching to this more difficult case. The central problem is that the model becomes a many-body system and so the Hilbert space grows quickly with system size. This renders an exact numerical calculation far beyond computational capabilities. Nevertheless, several studies have been accomplished, these suggest inclusion of interactions may yield non-trivial behaviour.

Shepelyansky³⁾ performed calculations on two interacting particles. In 1D, interactions caused a large enhancement of localization length. Other work showed that in 2D the effect is possibly stronger leading to delocalization.⁴⁾ However, some caution is required as the method fails to reproduce known non-interacting results when interactions are switched off.

The most successful method for treating the finite density problem is the Density Matrix Renormalization Group (DMRG) approach.⁶⁾ This works by performing a direct diagonalization but reducing the Hilbert space by systematically discarding basis states that do not contribute significantly to the ground state. Applying this method to the Anderson interacting model (defined in equation 1), a delocalized regime was found for attractive interactions.⁷⁾ In more recent papers by the same authors, it was noted that interesting physics is washed out in the averaging process. Charge reorganisations can be seen as electrons on a chain shift from the Mott insulator limit to (strong interactions) to the Anderson insulator limit (strong disorder).⁸⁾ Extensions of DMRG to 2D have encountered difficulties.

We have developed a new method incorporating some of the ideas of DMRG and the transfer matrix method successfully used in the non-interacting case.⁵⁾ Section 2 describes the method and section 3 discusses current progress.

2. A New Method

The method was developed using an interacting Anderson model:

$$\begin{aligned} \hat{H} = & \sum_i \epsilon_i \hat{c}_i^\dagger \hat{c}_i + V \sum_i (\hat{c}_i^\dagger \hat{c}_{i+1} + h.c.) \\ & + U \sum_i (\hat{c}_i^\dagger \hat{c}_i)(\hat{c}_{i+1}^\dagger \hat{c}_{i+1}) - \mu \sum_i \hat{c}_i^\dagger \hat{c}_i \end{aligned} \quad (1)$$

where \hat{c}_i^\dagger is the creation operator for site i . Site energies ϵ_i are chosen from a box distribution of width W . The hopping parameter is V and interaction strength given by U . The calculation is done in the grand canonical scheme with chemical potential μ .

The chain is grown by repeatedly adding sites to both ends. Given a set of eigenstates for a chain of length L , it is possible to form a basis for a chain of length $L+2$ by considering the possible occupancies of the two new end sites. An eigenstate $|\phi^L\rangle$ generates four basis states $|0\phi^L0\rangle$, $|1\phi^L0\rangle$, $|0\phi^L1\rangle$ and $|1\phi^L1\rangle$ where the 0 and 1 signify the occupancy of the two new end sites. Therefore, a general state of length $L+2$ and N electrons can be expanded as a linear combination of such basis states:

$$\begin{aligned} |\psi^{L+2,N}\rangle = & \sum_i a_i |0\phi_i^{L,N}0\rangle \\ & + \sum_j (b_j |1\phi_j^{L,N-1}0\rangle + c_j |0\phi_j^{L,N-1}1\rangle) \\ & + \sum_k d_k |1\phi_k^{L,N-2}1\rangle \end{aligned} \quad (2)$$

Note that particle number is a good quantum number so it is only necessary to expand in basis states where the total occupancy of $|\phi^L\rangle$ and the new sites is N . A Hamiltonian matrix may then be calculated for each particle number. This is done in the $L+2$ basis with the $|\phi^L\rangle$ eigenvalue on the diagonal plus elements due to addition of the end sites. Note that the eigenvectors of the

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system of length $L + 2$ are represented in the basis of the eigenvectors of the system of length L as expanded by the new sites. This implies that the calculation of the effective Hamiltonian for $L + 2$ sites is actually performed in the expanded basis of the eigenvectors for $L + 2$.

After calculating all the elements, the matrix is diagonalized with the eigenstates forming the basis states for the next iteration.

The approximation introduced to enable the calculation to fall within computational limits is to systematically remove basis states after each iteration. The simple approach is to retain the low energy states, as these are the only states likely to contribute to the next iteration ground state.

Most of the traditional methods for extracting the degree of localization do not carry across into the many-body case. Fortunately, phase sensitivity to boundary conditions does not suffer from this problem. This must be implemented as a perturbation because the calculation uses open boundary conditions. It turns out that this is equivalent to calculating off-diagonal elements of the reduced density matrix of the ground state, where the interior part of eigenstates is summed over. This is intuitively obvious because only the ends contain the relevant physics and we are interested in the probability of an electron entering one end and an electron appearing at the other. This procedure motivates simultaneously adding sites to both ends of the chain.

3. Preliminary Results

Initially, even in the non-interacting limit exponential decay was not observed in the middle of the band. However, it was found that this was an artifact of the particular criterium used for removing basis states. At first a set number of states was retained after each iteration, but this failed to reproduce exponentially localized behaviour even without interactions. It was then found this could be fixed by using a constant energy cutoff above the ground state and thereby allowing the number of states retained at each stage to fluctuate. However, the method still shows a significant dependence on the size of the energy cutoff and the number of states below the cutoff does not rise with system size as might be expected. We believe this to be due to the absence of the downward “pressure” of the eliminated states. We are currently investigating methods for compensating for this effect.

With these cautions, preliminary results have been obtained for the middle of the band (half filling). Schmitteckert⁸⁾ *et al* expected that repulsive interactions will enhance the effect of disorder, whereas attractive inter-

actions reduce it. Our preliminary results are in agreement with this (figure 1). Furthermore, a delocalized region for $U < -1$ was expected and observed using the DMRG method. The results presented here are consistent with this prediction, because our localization length diverges as U approaches -1 .

4. Conclusions

Further refinement of the Hilbert space reduction procedure is required before this method can be deemed re-

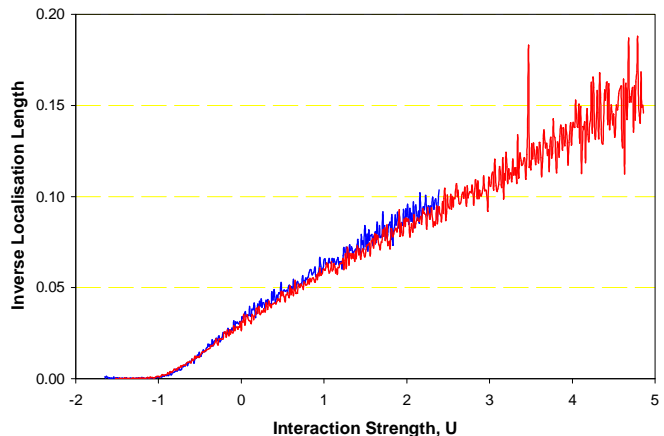


Fig. 1. Dependence of inverse localization length on interaction strength U in the middle of the band. Disorder $W = 2$, $V = 0$, $\mu = 0$. The average number of retained states at each step is 60 – continuous line, 80 – dotted line.

liable. Already extensions have been made for the Hubbard model and a double chain model. It is worth noting that the latter does not seem to suffer from the well-known sign problem.⁹⁾ It is hoped that this method can be eventually applied to the system with a finite cross section.

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